

# Does the side jump effect exist?

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The side-jump effect is a manifestation of the spin orbit interaction in electron scattering from an atom/ion/impurity. The effect has a broad interest because of its conceptual importance for generic spin-orbital physics, in particular the effect is widely discussed in spintronics. We reexamine the effect accounting for the exact nonperturbative electron wave function inside the atomic core. We find that value of the effect is much smaller than estimates accepted in literature. The reduction factor is  $1/Z^2$ , where  $Z$  is the nucleus charge of the atom/impurity. This implies that the side-jump effect is practically irrelevant for spintronics, the skew scattering and/or the intrinsic mechanism always dominate the anomalous Hall and spin Hall effects.

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There are two well known manifestations of the relativistic spin-orbit interaction in atoms; (i) spin orbital splitting of energy levels (fine structure) and (ii) right-left asymmetry in scattering (skew scattering) [1, 2]. The side jump effect is another manifestation of the spin-orbit interaction. The effective spin orbit interactions in solids, Luttinger Hamiltonian [3], Dresselhaus [4], Rashba [5] and Dzyaloshinskii-Moriya [6] interactions have the same origin as atomic fine structure. These lead to intrinsic spin-orbital effects irrelevant to a disorder/impurities in solids. Scattering of polarized electrons from impurities in a solid has a skew component completely analogous to that in atomic physics. This is an extrinsic spin-orbital effect.

Manipulation and detection of spins without magnetic field is one of crucial aspects in spintronics and can be done by the spin current [7]. By the spin Hall effect (SHE), the spin current can be generated from the charge current in a paramagnetic material without magnetic field and vice versa [8–12]. The SHE is similar to the anomalous Hall effect (AHE) in ferromagnetic materials. The spin-orbit interaction is necessary for both SHE and AHE (for review see Refs. [13–16]). The first mechanism for SHE proposed by Dyakonov and Perel [8] was the extrinsic one due to the skew scattering from impurities. Several intrinsic mechanisms have been also proposed [9, 10, 17, 18].

The side jump is another extrinsic mechanism for SHE and AHE. Remarkably, in spite of its generic importance, the effect is mostly unknown outside of spintronics community. The idea of the side jump effect was implicitly formulated in the pioneering work by Karplus and Luttinger [19]. Their approach has been further developed by Smit [20]. Among other mechanisms, Smit considered a possibility of the transverse jump of the wave packet. However, according to his analysis, this jump is equal to zero due to special kinematic cancellations. The idea

of the transverse coordinate jump of the wave packet was reintroduced by Berger, who has suggested the term “side jump” [21]. The theory of the side jump effect in its modern form was developed by Lyo and Holstein [22]. There are numerous discussions of the implications of the side jump effect (see Refs. [23–25]). It is worth noting some similarity between the side jump effect and Imbert-Fedorov effect in optics [26]. At a cartoon level, the idea

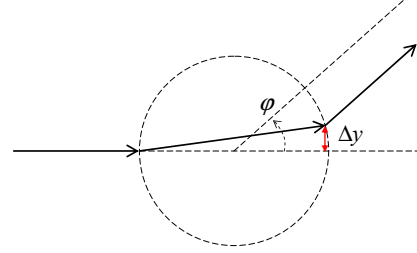


FIG. 1: Scattering of a polarized electron (polarization perpendicular to the plane) from impurity/atom/ion.  $\varphi$  is the skew scattering angle (right-left asymmetry) and  $\Delta y$  is the side jump displacement.

of side jump is explained in Fig. 1, which shows scattering of a polarized electron from an atom. The average deflection angle  $\varphi$  describes the skew scattering (right-left asymmetry) and the average displacement  $\Delta y$  is the side jump. Both the skew scattering and the side jump contribute to the multiple scattering deflection. As one might guess from the cartoon, the side jump can be significant compared to the skew only at a sufficiently high density of scattering centers when the mean free path is short.

For calculations, we adopt the Lyo & Holstein approach [22], in which the side jump transverse current is equal to the expectation value of the correction to the current operator due to the spin-orbit interaction. All previous calculations of the side jump effect were based on perturbation theory in the scattering poten-

tial. On the other hand, it is well known that such perturbation theory is not valid for atomic fine structure and for atomic skew scattering [1, 2]. The philosophy previously used for the side jump effect was to calculate the ratio of the side jump and the skew scattering within the perturbation theory and then to assume that nonperturbative effects do not change the ratio. In the present work, we demonstrate that this assumption is wrong. Intra-atomic nonperturbative effects suppress the ratio of the side jump over skew by orders of magnitude. The suppression factor is  $1/Z^2$ , where  $Z$  is the atom/impurity nuclear charge. This is because the skew scattering scales as  $\propto Z^2$  while the side jump is approximately  $Z$ -independent. Thus we conclude that the side jump mechanism is practically irrelevant even at high density of impurities, though the effect itself exists.

Consider the electron scattering from an impurity/atom. The Hamiltonian describing the problem is,

$$\begin{aligned} H &= H_0 + U_{ls}, \\ H_0 &= \mathbf{p}^2/2m + U(r), \\ U_{ls} &= \eta_{ls} \frac{1}{r} \frac{dU}{dr} (\mathbf{l} \cdot \mathbf{S}). \end{aligned} \quad (1)$$

Here  $U(r)$  is the impurity potential,  $\mathbf{l} = [\mathbf{r} \times \mathbf{p}]/\hbar$  and  $\mathbf{S}$  are orbital momentum and the spin of the electron, respectively. The parameter of spin-orbit interaction is denoted by  $\eta_{ls} = \hbar^2/(2m^2c^2)$  with the speed of light  $c$  and the electron mass  $m$ .

To illustrate scales involving in the problem, we present in Fig. 2 the self-consistent Hartree-Fock potential of Xe atom [27]. The typical spatial size of an atom/impurity is

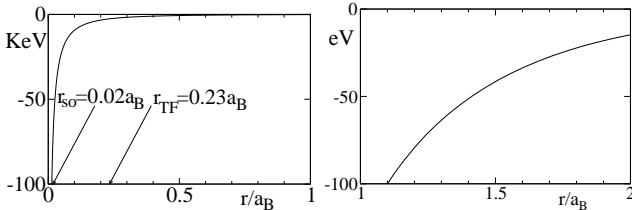


FIG. 2: Potential  $U(r)$  in Xe atom ( $Z = 54$ ). The left panel corresponds to  $r < a_B$  with the vertical scale given in KeV. The right panel corresponds to  $a_B < r < 2a_B$  with the vertical scale given in eV. Arrows in the left panel show the Thomas-Fermi and the spin-orbit scales.

a few Bohr radii,  $a \sim \text{few} \times a_B$ ,  $a_B = \hbar^2/(me^2) \approx 0.5 \text{ \AA}$ . The typical value of  $U(a)$  is about several eV. In Xe atom  $U(r = 2a_B) \approx -Ry$ , where  $Ry = (me^4/\hbar^2)/2 = 13.6 \text{ eV}$  is Rydberg. At  $r > a$  the potential quickly decays to zero due to electron screening. On the other hand, when  $r$  is decreasing,  $r < a$ , the potential grows strongly because of reduced screening. In Xe atom  $U(r = a_B) \approx -340 \text{ eV}$ . Below the Thomas-Fermi radius,  $r < r_{TF} = 0.885 a_B/Z^{1/3}$  [1], the potential grows even steeper,  $U(r) \approx -2ZRy(a_B/r)$ , because here nuclear charge is practically unscreened. This very singular

behavior of the potential is evident in Fig. 2. In the right panel,  $1 < r/a_B < 2$ , the potential is given in eV, while in the left panel,  $0 < r/a_B < 1$ , the potential is given in KeV.

It is well known [1] that all spin orbital effects originate from distances  $r \sim r_{so} = a_B/Z$ . This scale is indicated in the left panel of Fig. 2. At this distance, the potential is enormous,  $U(a_B/Z) = 2Z^2 Ry$  (which is 79 KeV for Xe), and the wave function behaviour is highly non-perturbative. This important fact was completely missing in all previous considerations of the side jump effect. In previous works the true very singular atomic potential was replaced by a soft nonsingular pseudopotential  $U(r) \rightarrow V(r)$  and calculations of both the skew scattering amplitude and the side jump were performed within simple perturbation theory in the pseudopotential  $V(r)$ . Any possible dependence on the nuclear charge  $Z$  was missing from the very beginning because there was no such a parameter in the analysis. On the other hand, it is clear that the nuclear charge is very important, because the spin orbit interaction is negligible in light atoms,  $Z \sim 1$ , and the interaction is much more significant in heavy atoms at  $Z \gg 1$ .

For low energy electrons,  $|\epsilon| \lesssim Ry$ , the spin-orbit energy splitting (fine structure) scales as  $Z^2$  [1]. We remind how this important statement is derived. Let us denote the electron wave function at  $r \sim a$  by  $\psi_0$ . A perturbative estimate of the effective spin-orbit interaction with a soft pseudopotential  $V(r)$  gives,

$$\begin{aligned} \langle \psi | \eta_{ls} \frac{1}{r} \frac{dV}{dr} (\mathbf{l} \cdot \mathbf{S}) | \psi \rangle &\sim \eta_{ls} \frac{Ry}{a_B^2} \langle \psi_0 | (\mathbf{l} \cdot \mathbf{S}) | \psi_0 \rangle \\ &\sim \alpha^2 Ry \langle \psi_0 | (\mathbf{l} \cdot \mathbf{S}) | \psi_0 \rangle, \end{aligned} \quad (2)$$

where  $\alpha = e^2/(\hbar c) = 1/137$  is the fine structure constant. Naturally, according to this estimate, the effective spin-orbit constant,  $\lambda \sim \alpha^2 Ry \sim 10^{-3} \text{ eV}$ , is very small and  $Z$ -independent. The true  $Z^2$  scaling is a nonperturbative effect. Because of the very strong potential, the electron wave function at  $r \sim r_{so} \sim a_B/Z$  is strongly enhanced compared to its exterior value [1] such as,

$$\psi(r) \sim \frac{\psi_0}{Z^{1/4} (r/a_B)^{3/4}}. \quad (3)$$

In particular  $\psi(r_{so}) \sim \sqrt{Z} \psi_0$ . Calculation of the matrix element of  $U_{ls}$  with the wave function (3) shows that the matrix element comes from the distances  $r \sim r_{so}$  and direct integration gives [1],

$$\langle \psi | U_{ls} | \psi \rangle \sim (Z\alpha)^2 Ry \langle \psi_0 | (\mathbf{l} \cdot \mathbf{S}) | \psi_0 \rangle. \quad (4)$$

Hence the effective spin-orbit constant is  $\lambda \sim (Z\alpha)^2 Ry$ . We disregard the  $l$ -dependence of  $\lambda$  ( $l$  is the angular momentum of the electron). The  $l$ -dependence can be easily included [28], but this is not important for our purposes. It is worth noting that due to the band structure the electron dispersion at low momenta is different from simple

parabolic one (1). Again, this is not important for us since at small distances (large momenta) relevant to the problem the dispersion is always quadratic.

The skew scattering is proportional to the scattering phase shift between the partial waves with total angular momenta  $j = l + 1/2$  and  $j = l - 1/2$  [1, 2]. Practically for electrons with  $\epsilon \lesssim Ry$  only  $l = 0, 1$  are important and the scattering cross section reads (assuming  $\delta_s \gg \delta_p$ )

$$\frac{d\sigma}{d\Omega} = \frac{d\sigma_0}{d\Omega} \{1 + 4(\delta_{p_{3/2}} - \delta_{p_{1/2}})(\mathbf{S} \cdot [\mathbf{n} \times \mathbf{n}'])\} , \quad (5)$$

where  $\frac{d\sigma_0}{d\Omega} = |f|^2$ ,  $f \sim a$  is the scattering amplitude without account of the spin-orbit interaction. Unit vectors  $\mathbf{n}$  and  $\mathbf{n}'$  are directed along initial and final electron momenta respectively. The phase shift can be calculated [1] using Eq. (4)

$$\delta_{p_{3/2}} - \delta_{p_{1/2}} \sim -\frac{ma^2}{\hbar^2} \langle \psi | U_{ls} | \psi \rangle \sim -(Z\alpha)^2 . \quad (6)$$

Therefore the skew cross section is

$$\frac{d\sigma}{d\Omega} = \frac{d\sigma_0}{d\Omega} \{1 - \gamma(Z\alpha)^2(\mathbf{S} \cdot [\mathbf{n} \times \mathbf{n}'])\} , \quad (7)$$

where  $\gamma \sim 1$  is a constant. Eqs. (6) and (7) are valid for electron energy above the centrifugal barrier. The barrier is always low as 1.8 eV in neutral Xe and zero in ions. Below the barrier, there is an additional centrifugal suppression,  $\delta_{p_{3/2}} - \delta_{p_{1/2}} \rightarrow (Z\alpha)^2(ka)^3$ , where  $k \ll 1/a$  is the wave vector of the electron. Eqs. (6) and (7) agree well with direct measurements for electron scattering from Xe [29].

Thus, similar to the fine structure splitting, the skew scattering scales as  $\propto Z^2$ . Therefore, it is important to know if the side jump has the same enhancement. The operator of the side jump velocity is

$$\delta \hat{\mathbf{v}}^{(sj)} = -\frac{i}{\hbar} [\mathbf{r}, H] - \frac{\mathbf{p}}{m} = \eta_{ls} [\mathbf{S} \times \nabla U] . \quad (8)$$

This operator is proportional to  $\nabla U = (\mathbf{r}/r)(dU/dr)$ . So, it has an additional power of the radius  $r$  compared to  $U_{ls}$  given by Eq. (1). Therefore, the straightforward *upper* estimate of the matrix element of Eq. (8) with the wave function (3) gives only the first power of  $Z$ , i.e.,  $\langle \delta \mathbf{v} \rangle \propto Z$ . Even this small result is an overestimate, due to exact equations of motion  $\langle \delta \mathbf{v} \rangle \propto Z^0 \sim 1$ . To prove this we represent  $\nabla U$  as

$$\nabla U = \frac{i}{\hbar} [\mathbf{p}, H_0] . \quad (9)$$

Hence to find the expectation value of  $\langle \delta \mathbf{v} \rangle$  from Eq. (8) we need to calculate the following matrix element in the limit  $\mu \rightarrow +0$

$$\frac{i}{\hbar} \langle \psi_{\mathbf{k}+} e^{-\mu r} [\mathbf{p}, H_0] e^{-\mu r} \psi_{\mathbf{k}+} \rangle . \quad (10)$$

Here  $\psi_{\mathbf{k}+}$  is the scattering state asymptotically,  $kr \gg 1$ , consisting of the incident plane wave and the diverging spherical wave,

$$\psi_{\mathbf{k}+} \rightarrow e^{i\mathbf{k} \cdot \mathbf{r}} + \frac{f}{r} e^{ikr} , \quad (11)$$

where  $f$  is the scattering amplitude. The parameter  $\mu \rightarrow +0$  is introduced to regularize the matrix element (10). This regularization is necessary for the wave-packet scattering problem to converge the integrals at  $r \rightarrow \infty$ . The matrix element (10) is calculated by commuting  $H_0$  with the regularization factor,

$$\begin{aligned} [H_0, e^{-\mu r}] &= [p^2/(2m), e^{-\mu r}] \\ &= \frac{i\mu\hbar}{2m} \left( \mathbf{p} \cdot \frac{\mathbf{r}}{r} e^{-\mu r} + e^{-\mu r} \frac{\mathbf{r}}{r} \cdot \mathbf{p} \right) . \end{aligned} \quad (12)$$

Hence, Eq. (10) is reduced to

$$-\frac{\mu}{m} \text{Re} \langle \psi_{\mathbf{k}+} \left| \left[ \left( \mathbf{p} \cdot \frac{\mathbf{r}}{r} \right) \frac{1}{r} e^{-\mu r} + e^{-\mu r} \frac{1}{r} (\mathbf{r} \cdot \mathbf{p}) \right] \mathbf{p} e^{-\mu r} \right| \psi_{\mathbf{k}+} \rangle . \quad (13)$$

Here “Re” stands for the real part. Importantly the expression (13) is proportional to the infinitesimally small  $\mu$ . Hence, the matrix element in Eq. (13) must be calculated only up to the order  $\mu^{-1}$ , all the higher orders,  $\mu^0$ ,  $\mu^1$ , ... will give zero contributions in the limit  $\mu \rightarrow 0$ . The terms proportional to  $1/\mu$  can appear only from large distances,  $r \sim 1/\mu$ . Hence, we can use the asymptotic form of the wave function (11) to calculate the matrix element in Eq. (13). Note that the wave function (11) is diverging at  $r \rightarrow 0$ . The divergence is a byproduct of the asymptotic form and therefore integrals of  $r$  in (13) have a lower cutoff of the order of atomic size. All the terms which are sensitive to the value of the cutoff disappear in the limit  $\mu \rightarrow 0$ .

Here, one can notice two interesting points. The side jump current, which is equal to the matrix element of Eq. (8), flows at very small distances from the nucleus,  $r \sim r_{so} \sim a_B/Z$ . Nevertheless the exact equation of motion (9) allows us to translate calculation of the integrated side jump current to the large distances,  $r \sim 1/\mu \rightarrow \infty$ . The second point concerns the infrared regularization  $\mu$ . The first order perturbation theory calculation ( $U(r)$  is the perturbation), which was performed in Ref. [22], also uses an infrared regularization by doing the substitution  $1/(\epsilon - \epsilon_k) \rightarrow 1/(\epsilon - \epsilon_k + i\mu) \rightarrow -i\pi\delta(\epsilon - \epsilon_k)$ . Our regularization method (13) is exact, and does not refer to the perturbation theory. We cannot rely on the perturbation theory, since we account all orders in  $U(r)$ .

In the order of  $1/\mu$ , the both terms in the square brackets in Eq. (13) give equal contributions and Eq. (13) is transformed to

$$\frac{\hbar^2}{m} \left\{ 4\pi k \text{Im} f(0, 0) \mathbf{n} - k^2 \int d\Omega |f(\theta, \varphi)|^2 \mathbf{n}' \right\} . \quad (14)$$

We remind that  $\mathbf{n} = (0, 0, 1)$  is the unit vector along momentum of the incident electron,  $f(\theta, \varphi)$  is the scattering amplitude,  $d\Omega$  is the scattering solid angle, and  $\mathbf{n}' = (\sin\theta \cos\varphi, \sin\theta \sin\varphi, \cos\theta)$  is the unit vector in the scattering direction. Due to the optical theorem the imaginary part of the forward scattering amplitude is related to the total cross section [1],

$$\text{Im}f(0, 0) = \frac{k}{4\pi}\sigma_0 = \frac{k}{4\pi} \int d\Omega |f(\theta, \varphi)|^2. \quad (15)$$

Here the scattering amplitude  $f$  and the scattering cross section  $\sigma_0$  are calculated without account of the spin-orbit interaction. We remind that while we treat the interaction potential *exactly*, the spin-orbit interaction is considered only in the first order. Hence Eq.(14) is transformed to the transport cross section and we obtain the following relation

$$\langle \psi_{\mathbf{k}+} | \nabla U | \psi_{\mathbf{k}+} \rangle = \mathbf{k} \frac{\hbar^2 k}{m} \sigma_{tr} = \hbar \mathbf{k} v \sigma_{tr} \quad (16)$$

$$\sigma_{tr} = \int (1 - \cos\theta) |f(\theta, \varphi)|^2 d\Omega,$$

where  $v$  is speed of the electron. This equation represents the force-momentum balance, i.e., the average force acting on the atomic nucleus (the left hand side of Eq. (16)) is equal to the momentum transfer from the incident electron beam (the right hand side of Eq. (16)). Because of this reasoning, one can skip the technical derivation of Eqs.(9)-(15) and go straight to Eq. (16).

Taking the matrix element of Eq. (8) over the state  $\psi_{\mathbf{k}+}$  and using the exact relation (16) we find

$$\langle \delta \mathbf{v}^{(sj)} \rangle = \eta_{ls} [\mathbf{S} \times \mathbf{k}] v \sigma_{tr}. \quad (17)$$

This is similar to the result in Ref. [22]. However (17) has been derived exactly for arbitrary strong potential of a heavy atom. The most important issue is that the side jump (17) does not scale with nuclear charge  $Z$ , while the skew scattering (7) scales as  $Z^2$  (see comment [30]).

The spin Hall conductivity  $\sigma_{xy}$  is defined by equation  $J_{sy} = \sigma_{xy} E_x$ , where  $J_{sy}$  is the  $y$ -component of spin current and  $E_x$  is the  $x$ -component of electric field. The ratio of the side jump (SJ) contribution and the skew scattering (SS) contribution to the conductivity was calculated in Ref. [31] within the perturbation theory. Using solution of the kinetic equation from Ref. [31], and using exact Eqs. (7) and (17) instead of the corresponding perturbative Eqs. in Ref. [31], we find

$$\frac{\sigma_{xy}^{SJ}}{\sigma_{xy}^{SS}} \sim \frac{1}{Z^2} \frac{\hbar}{\tau_{tr} R y}. \quad (18)$$

Thus, even in the most dirty metal where  $\frac{\hbar}{\tau_{tr} R y} \sim 1$ , the side jump contribution to the spin Hall conductivity is suppressed compared to that of the skew scattering by the factor  $1/Z^2$ .

*In conclusion.* The skew scattering from an impurity/atom (the right-left asymmetry) is a spin-orbital effect enhanced by the nuclear charge of the impurity  $\propto Z^2$ . The side jump effect is another manifestation of the spin-orbit interaction in electron scattering from impurities/atoms. We have demonstrated that due to the complex intra-atomic structure of the electron wave function the side jump effect is not enhanced by  $Z$  contrary to the view accepted previously. This implies that relative to the skew the side jump effect is smaller by the factor  $1/Z^2$  compared to all previous estimates. For typical semiconductors,  $Z \sim 30 - 50$ , the suppression factor is about  $\sim 10^3$ . This makes the side jump effect irrelevant compared to the skew scattering even in most dirty materials.

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